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(Volume A)

FINAL REPORT

COVERING THE PERIOD
20 MARCH 1961-31 MAY 1962

Title: METHODS IN MONTE CARLO SOLUTION OF THE RADIATION TRANSPORT EQUATION

Prepared by
M. H. Kalos

Date: 31 May 1962

Contract No.: DA-18-108-405-CML-1007 (Project 2167)

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ABSTRACT

A discussion is given of certain methods of importance sampling and scoring in the Monte Carlo solution of the radiation transport equation.

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1. INTRODUCTION

In the spring of 1961, the Development Division of United Nuclear Corporation, with the sponsorship of the U.S. Army Nuclear Defense Laboratory, undertook a study aimed at the preparation of a comprehensive radiation transport program. A survey was made of existing codes capable of yielding information on the penetration of neutrons and gamma rays in the atmosphere following a nuclear weapons detonation. In addition, information was obtained from individuals interested in weapons effects on the type and range of answers needed.

On the basis of these surveys, a set of recommendations was prepared for the new program.[1] In addition, flow charts for portions of the code were prepared. When, however, the Los Alamos Scientific Laboratory volunteered to prepare the actual machine program for the STRETCH computer, the United Nuclear activity was redirected so as to provide support to Los Alamos. This support has been in the areas of investigation of Monte Carlo techniques and the preparation of neutron cross sections for the program.

The latter activity is reflected in the second part of this report (Volume B) which contains a set of cross section information for Be^9.

This part of the report is a description of studies of certain topics related to the Monte Carlo solution of the transport equation. A really comprehensive solution, as now planned, will tax the speed of the fastest present computer so that methods of improving the computational efficiency are needed.

In undertaking to provide possible methods, we have assumed, not quite correctly, that the problem of designing the computation procedure may be split

into two or three separate problems. The first of these is concerned with importance sampling, taken up in Section 2. This is understood to mean, for our purposes, altering the natural history of a neutron or gamma ray so as to insure an adequate supply of collisions even at large distances from the source. We assume that the blast wave and similar complications have no essential role in designing the importance sampling.

The second problem, with which Section 3 is concerned, is that of scoring. This means using the collisions which make up the histories to get answers of any desired kind. Considerable emphasis is placed upon efficient means of computing flux or dose at a point. Finally, Section 4 is devoted to a discussion of methods of eliminating unncessary flux calculations when there are many detectors.

Although the work cannot be considered complete until the methods are tried out in the final code or a similar one, specific recommendations are made for importance sampling and scoring in Sections 2 and 3. The material in Section 4 has not been completed to the point where a recommendation can be made; however, the method may be introduced easily into any code.

Finally, considerable work remains in reducing the methods proposed to practical flow charts for coding into the transport calculation.

2. IMPORTANCE SAMPLING

2.1 GENERAL THEORY

In order to discuss the aims and problems of importance sampling, let us review the basic theory. Write the integral Boltzmann equation for $\chi(\underset{\sim}{P})d\underset{\sim}{P}$, the density of particles coming out of collision in $d\underset{\sim}{P}$ (in phase space) as

$$\chi(\underset{\sim}{P}) = \int K(\underset{\sim}{P}'\rightarrow\underset{\sim}{P})\,\chi(\underset{\sim}{P}')d\underset{\sim}{P} + S(\underset{\sim}{P}). \tag{2.1}$$

$K(\underset{\sim}{P}'\rightarrow\underset{\sim}{P})\,d\underset{\sim}{P}$ is the expected number emerging from a collision at $\underset{\sim}{P}$ in $d\underset{\sim}{P}$, given that a particle came out of collision at $\underset{\sim}{P}'$. $S(\underset{\sim}{P})$ is the source density. Eq. 2.1 may be transformed with the use of an arbitrary positive function $I(\underset{\sim}{P})$. Multiply through by the factor

$$\frac{I(\underset{\sim}{P})}{\int I(\underset{\sim}{P})\,S(\underset{\sim}{P})\,d\underset{\sim}{P}}$$

and define

$$\tilde{\chi} = \frac{\chi(\underset{\sim}{P})\,I(\underset{\sim}{P})}{\int I(\underset{\sim}{P}')\,S(\underset{\sim}{P}')\,d\underset{\sim}{P}'} \tag{2.2}$$

$$\tilde{\chi}(\underset{\sim}{P}) = \int K(\underset{\sim}{P}'\rightarrow\underset{\sim}{P})\frac{I(\underset{\sim}{P})}{I(\underset{\sim}{P}')}\,\chi(\underset{\sim}{P}')\,d\underset{\sim}{P}' + \frac{S(\underset{\sim}{P})\,I(\underset{\sim}{P})}{\int S(\underset{\sim}{P})\,I(\underset{\sim}{P})\,d\underset{\sim}{P}} \tag{2.3}$$

This equation is the same, formally, as Eq. 2.1, with a new normalized source distribution, and a new kernel

$$\tilde{K}(\underset{\sim}{P}'\rightarrow\underset{\sim}{P}) = \frac{I(\underset{\sim}{P})}{I(\underset{\sim}{P}')}\,K(\underset{\sim}{P}'\rightarrow\underset{\sim}{P}) \tag{2.4}$$

Suppose that a single answer of the form

$$\langle f \rangle = \int \chi(\underset{\sim}{P})\, f(\underset{\sim}{P})\, d\underset{\sim}{P} \tag{2.5}$$

is required. Then it can be shown[3] that a particular choice of $J(\underset{\sim}{P})$ satisfying the adjoint equation

$$J(\underset{\sim}{P}) = \int K(\underset{\sim}{P} \rightarrow \underset{\sim}{P}')\, J(\underset{\sim}{P}')\, d\underset{\sim}{P}' + f(\underset{\sim}{P}) \tag{2.6}$$

used for $I(\underset{\sim}{P})$ permits the answer (Eq. 2.5) to be obtained exactly (i.e., with zero variance).

The function $J(\underset{\sim}{P})$, the "importance function," has the physical meaning of the expected final contribution to the required answer $\langle f \rangle$ for a particle coming out of collision at $\underset{\sim}{P}$. The altered kernel has the reasonable property that it should be biased to encourage collisions where they are likely to give significant contributions to the answers. Beyond trying to exploit this last feature importance sampling is not often carried out because of the following difficulties.

1. $J(\underset{\sim}{P})$ is never known exactly. If it were then the identity

$$\int J(\underset{\sim}{P})\, S(\underset{\sim}{P})\, d\underset{\sim}{P} = \int f(\underset{\sim}{P})\, \chi(\underset{\sim}{P})\, d\underset{\sim}{P} \tag{2.7}$$

would permit solution by quadrature. Solution of the adjoint equation is as difficult as solution of the original equation. However, it has been argued[3] that since the variance is positive, a choice $I(\underset{\sim}{P})$ which has the essential features of $J(\underset{\sim}{P})$ may make the variance very small. The physical meaning of $J(\underset{\sim}{P})$ can often be used to help estimate a "reasonable" guess of $I(\underset{\sim}{P})$.

2. If we attempt to use an $I(\underset{\sim}{P}) \approx J(\underset{\sim}{P})$ the normalization of the kernel (Eq. 2.4) is unknown. That is

$$N(\underset{\sim}{P}') = \int d\underset{\sim}{P}\, K(\underset{\sim}{P}' \rightarrow \underset{\sim}{P})\, \frac{I(\underset{\sim}{P})}{I(\underset{\sim}{P}')} \tag{2.8}$$

can not be evaluated in closed form and the expected number of particles emerging from all collisions can not be evaluated. This difficulty can be evaded in two ways. One is to use an I such that the integral (Eq. 2.8) can be evaluated. The exponential transformation may be regarded as such a choice. Another is to

form any kernel $K'(\underset{\sim}{P}' \to \underset{\sim}{P})$ which is similar to $\tilde{K}(\underset{\sim}{P}' \to \underset{\sim}{P})$, pick from K', evaluate

$$N' = \frac{\tilde{K}(\underset{\sim}{P}' \to \underset{\sim}{P})}{K'(\underset{\sim}{P}' \to \underset{\sim}{P})}$$

and create this number of particles coming out of collision at $\underset{\sim}{P}$. This generalization of the usual splitting and Russian roulette may, in turn, be carried out in several ways. If we put $K' = K$, then the procedure is simply to track particles in the usual (unbiased) way from collision to collision and create $I(\underset{\sim}{P})/I(\underset{\sim}{P}')$ particles for each one that comes out of collision at $\underset{\sim}{P}$. This is simple and direct, but it has the disadvantage that the important parts of phase space are encountered rarely (if we have to resort to importance sampling at all). Then the result is to create many particles very infrequently – a procedure that is characterized by a large variance.

A somewhat more sophisticated procedure in which an effort was made to approximate $\tilde{K}$ has been carried out successfully[4] and shown to permit the reliable computation by Monte Carlo methods of penetration through very deep layers.

3. In many problems, there is no single answer of primary interest. On the contrary, a map of the radiation field as a function of position, energy, and time may be desired. If importance sampling is carried out as outlined above, one particular answer (e.g., at the deepest penetration) may be estimated well at the expense of accuracy of the others.

If importance sampling could be designed very well, then it may happen that a set of different estimates of the same radiation field may be better obtained by separate computations with different biasing. It is likely, for instance, that secondary gamma sources in the atmosphere are best derived from unbiased neutron histories separate from those used to give deep neutron penetration.

On the other hand, if we assume that it is not possible to design the importance sampling so that individual answers are given very precisely, it is desirable to introduce an importance function which gives reasonably good estimates for detectors spread throughout space. We suppose that these detectors are located

in the vicinity of $\underset{\sim}{r}_i$, i = 1, 2, ... , and that the total flux, integrated over time and energy, is to be estimated with a given precision at each one. The last assumption does not preclude the possibility of recording time and energy dependence. What it means is that where, at a given position, the flux is small at some time as compared with a different time, that we will be content with the lower precision attached to the estimate of the smaller flux.

For purposes of importance sampling, we ask that the several fluxes be estimated in such a way that the weighted sum

$$\langle f \rangle = \Sigma\, w_i \phi(\underset{\sim}{r}_i) \tag{2.9}$$

is estimated with minimum variance. If we wish to estimate the fluxes so that each has approximately a constant relative error, then

$$w_i \propto [\phi(\underset{\sim}{r}_i)]^{-1}. \tag{2.10}$$

More specifically, we should make w_i inversely proportional to the total expected contribution from which a flux value is deduced. For example, suppose that we wish to estimate the flux in a number of spherical shells of constant thickness placed about a point source of radiation. Then for each shell an integral proportional to $4\pi r^2 \phi$ is obtained, the prescription for weighting is then that we should set

$$w = \frac{1}{4\pi r^2 \phi}$$

which, in turn, may be estimated roughly as

$$w \approx e^{\mu_0 r}.$$

Since we wish to obtain fluxes weighted by w, it is reasonable to use w as an importance function, I.

It is worth re-emphasizing that this choice of importance function derives primarily from the desire to estimate fluxes with approximately constant relative error <u>throughout</u> a certain range, rather than a desire to obtain penetration through a shield.

2.2 AN EXPONENTIAL TRANSFORMATION FOR SPHERICAL GEOMETRY

Let us illustrate the general notions of the preceding paragraph with a somewhat simplified, although useful, example. Consider the transport in a homogeneous infinite medium with a point source. The spatial dependence of the flux is through the radial distance, r, alone.

To carry out importance sampling with an importance function

$$I = e^{\mu_0 r} \tag{2.11}$$

we split the kernel $K(\underset{\sim}{P}' \to \underset{\sim}{P})$ into a "transport" and a "collision" kernel:

$$K(\underset{\sim}{P}' \to \underset{\sim}{P}) = T(\underset{\sim}{r}' \to \underset{\sim}{r} \mid E', \underset{\sim}{\Omega}')C(E' \to E, \underset{\sim}{\Omega}' \to \underset{\sim}{\Omega} \mid \underset{\sim}{r}) \tag{2.12}$$

where T gives the expected number of particles going into collision in $d\underset{\sim}{r}$ at $\underset{\sim}{r}$ given that a particle came out of collision at $\underset{\sim}{r}'$ with energy E', direction $\underset{\sim}{\Omega}'$; C gives the expected number of particles coming out of collision at $\underset{\sim}{r}$ with energy in dE, direction in $d\underset{\sim}{\Omega}$, given that one went into collision with $E', \underset{\sim}{\Omega}'$. With an importance function that depends upon position only, the altered kernel

$$\tilde{K}(\underset{\sim}{P}' \to \underset{\sim}{P}) = \frac{I(\underset{\sim}{P})}{I(\underset{\sim}{P}')} K(\underset{\sim}{P}' \to \underset{\sim}{P}) \tag{2.13}$$

requires a change in the transport kernel only:

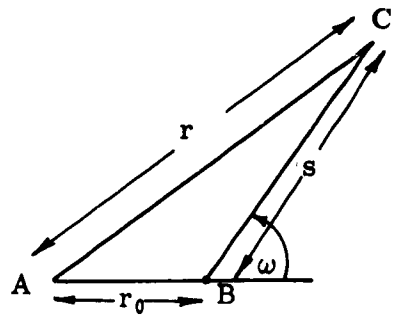
$$\tilde{K} = \tilde{T} C \tag{2.14}$$

$$\tilde{T} = \frac{I(\underset{\sim}{r})}{I(\underset{\sim}{r}')} \quad T(\underset{\sim}{r}' \to \underset{\sim}{r} \mid E', \underset{\sim}{\Omega}) \, . \tag{2.15}$$

It is now necessary to establish a random walk whose transport kernel is given by $\tilde{T}$.

It has been pointed out that this is, to a large extent, arbitrary. One method, for example, is to follow particles from $\underset{\sim}{r}'$ to $\underset{\sim}{r}$ using the kernel T, and then create, on the average, $I(\underset{\sim}{r})/I(\underset{\sim}{r}')$ particles going into collision at $\underset{\sim}{r}$. This method, a generalization of splitting and Russian roulette, is easy to carry out. It has the important disadvantage that when a particle flies radially outward, then, with low

probability many particles are created. Thus additional variance, which may be large, is associated with the spliting process. It is desirable to use a kernel as close to $\tilde{T}$ as can be arranged conveniently.



For the spherical problem under discussion, the appropriate geometry is sketched in the figure.

Suppose a particle starts a flight at B, in a direction whose cosine is ω with respect to the radius from the source. The original transport kernel is given by the conditions that

a. The next collision is along the ray BC.

b. The expected number of collisions in ds at s is given by

$$T(s)\,ds = \mu(E')\, e^{-\mu(E')s}\, ds \tag{2.16}$$

where $\mu(E') \equiv \mu'$ is the macroscopic cross section at energy E'.

With the importance function

$$I = e^{\mu_0 r}$$

the altered transport kernel satisfies (a) above, but (b) is replaced by

$$\begin{aligned}\tilde{T}(s) &= T(s)\, e^{\mu_0 r(s) - \mu_0 r_0} \\ &= \mu' \exp(-\mu' s + \mu_0 \sqrt{r_0^2 + 2r_0\omega s + s^2} - \mu_0 r_0) \\ &\equiv \mu' \exp[-\lambda(s)] \end{aligned} \tag{2.17}$$

This kernel is not easy to pick from (for one thing it is not normalized to give exactly one next collision). It is straightforward, however, to pick from the kernel

$$T'(s) = + \frac{d\lambda(s)}{ds} \exp\left[-\lambda(s)\right]. \tag{2.18}$$

To do it, pick λ_0 from the p.d.f. $e^{-\lambda}$ and determine s_0 from

$$\lambda(s_0) = \lambda_0$$

The solution for s_0 is

$$s_0 = \frac{\lambda_0\mu' - \mu_0(\mu' - \omega\mu_0)r_0 + \mu_0\left[(\mu' - \omega\mu_0)^2 r_0^2 + 2(\omega\mu' - \mu_0)\lambda_0 r_0 + \lambda_0^2\right]^{1/2}}{\mu'^2 - \mu_0^2} \tag{2.19}$$

and

$$r = (r_0^2 + 2\omega r_0 s_0 + s_0^2)^{1/2}$$

$$= r_0 + \frac{\mu'}{\mu_0} s_0 - \frac{\lambda_0}{\mu_0} \tag{2.20}$$

In doing this we assume that $\mu' > \mu_0$. This is not, of course, a necessary assumption. To relax it, however, it is necessary to be more careful about the behavior of the importance function for large r and to take care to calculate s_0 correctly when $\mu' \approx \mu_0$.

Having picked s from a kernel other than $\tilde{T}$, it is necessary to arrange that N particles go into collision where

$$N = \frac{\tilde{T}}{T'} = \frac{\mu'}{\frac{d\lambda}{ds}} \tag{2.21}$$

But

$$\frac{d\lambda}{ds} = + \mu' - \frac{\mu_0(s + r_0\omega)}{\sqrt{r_0^2 + 2r_0\omega s + s^2}} = +\mu' - \frac{\mu_0(s + r_0\omega)}{r}$$

$$N = \frac{\mu' r}{\mu' r - \mu_0 s_0 - \mu_0 \omega r_0} \tag{2.22}$$

Since

$$\mu' > \mu_0$$

and

$$r \geq s + \omega r_0$$

we have

$$\frac{\mu'}{\mu'-\mu_0} \geq N > 0 \qquad (2.23)$$

The factor N can be used as a weight factor or as a particle multiplication factor. The latter seems more natural. In a straight ahead, one-velocity transport problem in which the absorption probability is 1-C, the flux behaves like

$$4\pi r^2 \phi = \exp\left[-(1-C)\ \mu' r\right]$$

It is natural to take $\mu_0 = (1-C)\mu$; for which

$$N = \frac{\mu'}{\mu' C} \ .$$

Hence, if N is taken to be a particle splitting factor as discussed here, the expected number of particles coming out of collision is NC = 1. In this simple problem, suppression of absorptions comes about in a natural way. We suppose that in a real spherical calculation that the same behavior will hold at least qualitatively and that N should be used to create extra particles rather than as a weight factor. Naturally, it is best to compute $N\ \mu_S/\mu_T$ at the next collision and arrange that this many particles come out of collision there.

The exponential transformation for spherical geometry that has been discussed here may be generalized to concentric spherical shells. It will not be discussed further, since it has been included primarily for purposes of illustration. The geometrical complication associated with the inhomogeneous atmosphere makes it impossible to carry out importance sampling this well. Before discussing the atmosphere question in detail, we carry out a further simplification of the spherical problem which suggests a simple treatment of the atmosphere importance sampling. This involves making, in Eq. 2.17, the two limiting approximations for small and large s:

$$r = \sqrt{s^2 + 2\omega r_0 s + r_0^2}$$

$$\approx r_0 + \omega s \qquad s << r_0$$

$$\approx s + \omega r_0 \qquad s >> r_0 \tag{2.24}$$

These are exactly right when $\omega = \pm 1$ and otherwise underestimate r by, at most, $1/2\ r_0$. We propose to use these approximations in $\tilde{T}$ to obtain a T''.

$$T'' = \frac{d\lambda_i}{ds} \exp\left[-\lambda_1(s)\right] \tag{2.25}$$

$$\begin{aligned} \lambda_1(s) &= \mu' s - \mu_0 r_0 - \mu_0 \omega s + \mu_0 r_0 \qquad s \leq r_0 \\ &= \mu' s - \mu_0 s - \mu_0 \omega r_0 + \mu_0 r_0 \qquad s > r \end{aligned} \tag{2.26}$$

To pick from T'', let λ_0 be chosen from $e^{-\lambda}$ and if

$$\lambda_0 \leq (\mu' - \omega\mu_0) r_0; \qquad s = \frac{\lambda_0}{\mu' - \omega\mu_0}$$

if (2.27)

$$\lambda_0 > (\mu' - \omega\mu_0)\ r_0; \qquad s = \frac{\lambda_0 - \mu_0(1-\omega) r_0}{\mu' - \mu_0}$$

Effectively, these correspond to carrying out the exponential transformation for the plane for $s < r_0$, and assuming a straight ahead approximation for $s > r_0$. N is now computed as

$$\begin{aligned} N'' &= \frac{\mu'}{\mu' - \omega\mu_0} \exp\left[\mu_0(r - r_0) - \mu_0 \omega s\right]; \qquad s \leq r_0, \\ &= \frac{\mu'}{\mu' - \mu_0} \exp\left[\mu_0(r - s - \omega r_0)\right]; \qquad s > r_0 \end{aligned} \tag{2.28}$$

$$r = (r_0^2 + 2\omega r_0 s + s^2)^{1/2}$$

Wells[5] has suggested using the first part of Eq. 2.27 alone in spherical problems.

2.3 IMPORTANCE SAMPLING IN AN INHOMOGENEOUS ATMOSPHERE

The change in atmospheric density with altitude complicates any attempt at importance sampling in two ways; as we have seen, it is necessary to introduce a guess at the nature of the solution and this is more difficult. Carrying out the implied importance sampling is also more involved.

A relatively straightforward method of importance sampling follows if we subdivide space into a large number of finite volumes. For an atmosphere in which the density depends only upon vertical height, these volumes may be defined by the intersection of horizontal planes and concentric cylinders with a vertical axis. We assume an importance function which is piece-wise constant in each of these volumes. The values may be computed to be inversely proportional to an integrated flux as indicated in the preceding section. On the other hand, the values may be chosen so as to emphasize regions of space close to particular detectors.

In any case, this importance function may be used to define a splitting-and-Russian-roulette procedure: when a particle is tracked from a volume in which the importance function is I_1 to a volume in which it is I_2, arrange that

$$N = I_2/I_1$$

particles, on the average actually enter the new region. If $N < 1$, N is interpreted as a probability of continuing the history (1-N is the probability of Russian roulette). If $N > 1$, compute the integer part $\{N\}$ and fractional part $N-\{N\}$ respectively. Arrange that $\{N\}$ plus with probability $N-\{N\}$ one more particles actually enter the region. This is usually done by following one particle, and entering coordinates of the remaining particles in a "latent" list. The particles in a "latent" list are taken up one at a time after the preceding parts of a history are terminated in the usual way.

This splitting provides a very flexible and straightforward way of increasing particle populations in otherwise unlikely parts of space. It has been used successfully in a number of applications.

The disadvantages of the method are as follows. First, for the atmosphere problem, it requires the introduction of an otherwise extraneous geometry with the necessity of tracking through it. Second, it requires the specification of the many values of the importance function. Third, the process of splitting introduces additional variance. The third objection should not be understood to mean that splitting is not worthwhile, but that alternative ways of using the importance function may be better.* The second objection may be overcome if an analytic computation of the importance function can be devised.

In view of these disadvantages, especially the first, we have given some attention to the possibility of devising an alternative scheme, more nearly along the lines of the earlier section. The first part of such a scheme requires the specification of a simple approximate form for the importance function.

A simple generalization of the radial exponential is

$$I(\underset{\sim}{r}) = \exp\left[\sigma_0 \int \rho(s)\, ds\right] \tag{2.29}$$

where the integral of the density is taken along the line from source to point $\underset{\sim}{r}$. We introduce the cumulative density function

$$F(z) = \int_z^\infty \rho(z)\, dz \tag{2.30}$$

where z is vertical height and $\rho(z)$ is the atmospheric density at z. Let $\underset{\sim}{r}$ be specified by (x,y,z) and

$$\gamma = z/r = z(x^2+y^2+z^2)^{-1/2} \tag{2.31}$$

$$I(x,y,z) = \exp\left\{\frac{\sigma_0}{\gamma}\left[F(z_0) - F(z)\right]\right\} \tag{2.32}$$

*One such method has been proposed: it consists in examining the segments cut off the particle path by the volume subdivision, and computing the expected number of particles which should go into collision in each segment. This number is given by $(I \int \mu e^{-\mu s} ds)$ for each segment. One arranges that this number, on the average, go into collision in that segment. The method has the apparent advantage that long flights do not depend upon the survival of a cascade through the shorter distances. It has not been tried to any extent.

where the source is at $(0,0,z_0)$. The value of σ_0 is adjustable.

This form of the importance function must be regarded as tentative. It is reasonable when the variation in density is not large since it reduces to $\exp(-\sigma_0 r)$ in that case. For very large distances when the density is rapidly varying it may well be wrong. For example, it may be easiest to achieve deep penetration by a flight to a thin part of the atmosphere, followed by a long flight through this region. An "indirect" penetration of this kind is not properly emphasized by the importance function.

The validity of the proposed function has been tested in two ways. First, very crude multiple scattering calculations were made to see whether an indirect flight can lead to much larger fluxes at great distances than a direct flight. In these calculations distances were chosen so that 0.1 rad would result from a 100 megaton yield. This pushes the parameters to their limit. An effective attenuation coefficient of 0.04 cm^2/g was used throughout. Multiple scattering in volumes about one mean free path on a side was estimated for various positions of source and scattering volumes. According to the rough estimates obtained, the indirect scattering can exceed the direct flux when the source is above 12 km. Even at the extreme ranges, the excess is, at most, a factor of 100. This ratio is, of course, very important itself, but is not considered to be a serious error in designing an importance function.

A second check on the flux estimate was made by plotting $4\pi r^2\phi$ vs $\int\rho ds$ from some calculations already made of penetrations in the atmosphere. These calculations may not be entirely reliable at very deep penetrations, since no importance sampling was involved.

In Figs. 2.1 and 2.2 the results for total flux in the highest energy bins are plotted for two source energies, two source heights, and several detector positions. The points do not fall far from straight lines, indicating again that the flux form in Eq. 2.29 is reasonable. The reason for the difference in slopes between the "DOFL" and "SANDIA" curves in Fig. 2.2 in unknown, but is presumed to result from different cross sections.

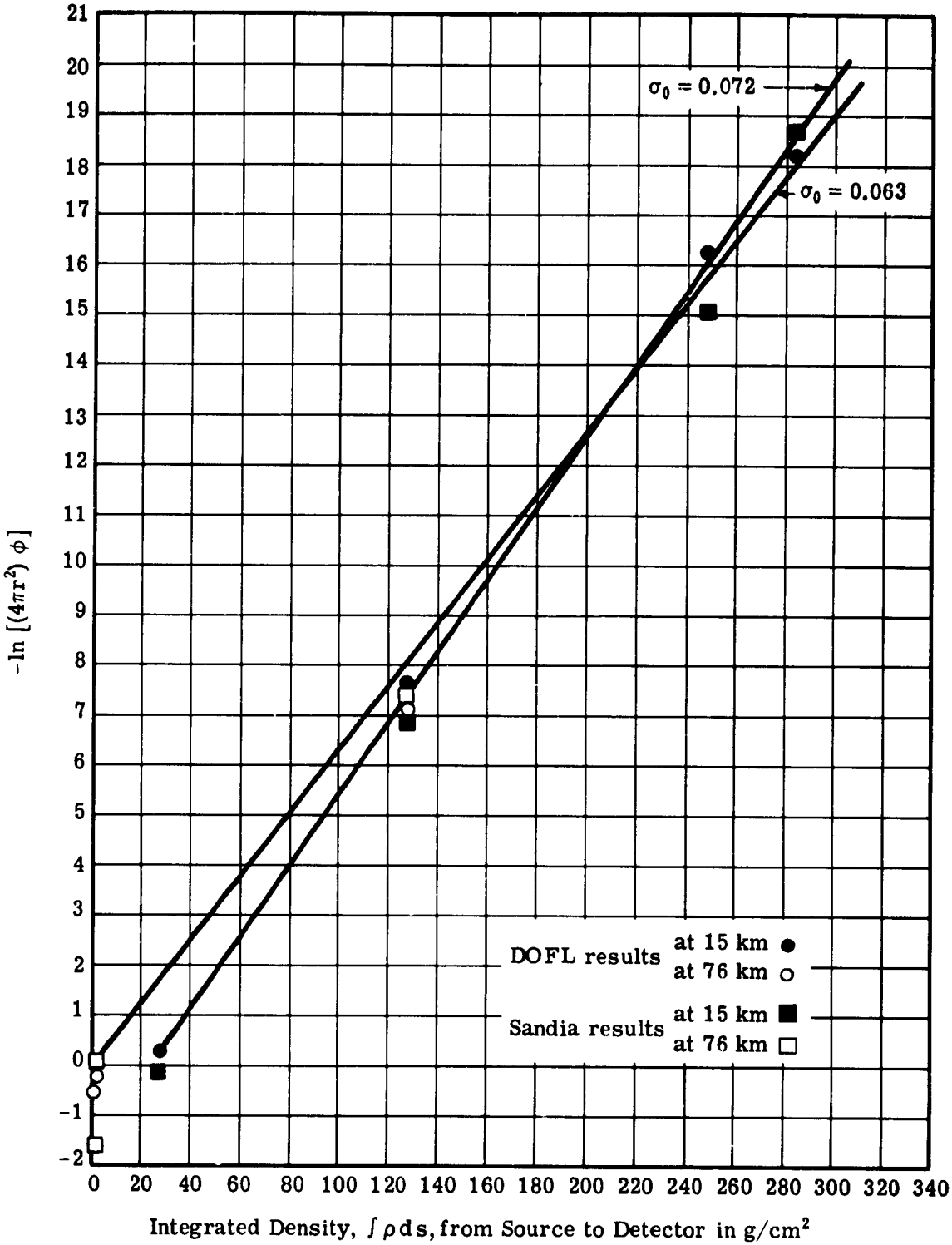


Fig. 2.1 — Neutron penetration in the atmosphere; flux of 1.5 to 2 Mev neutrons from a 2-Mev source.

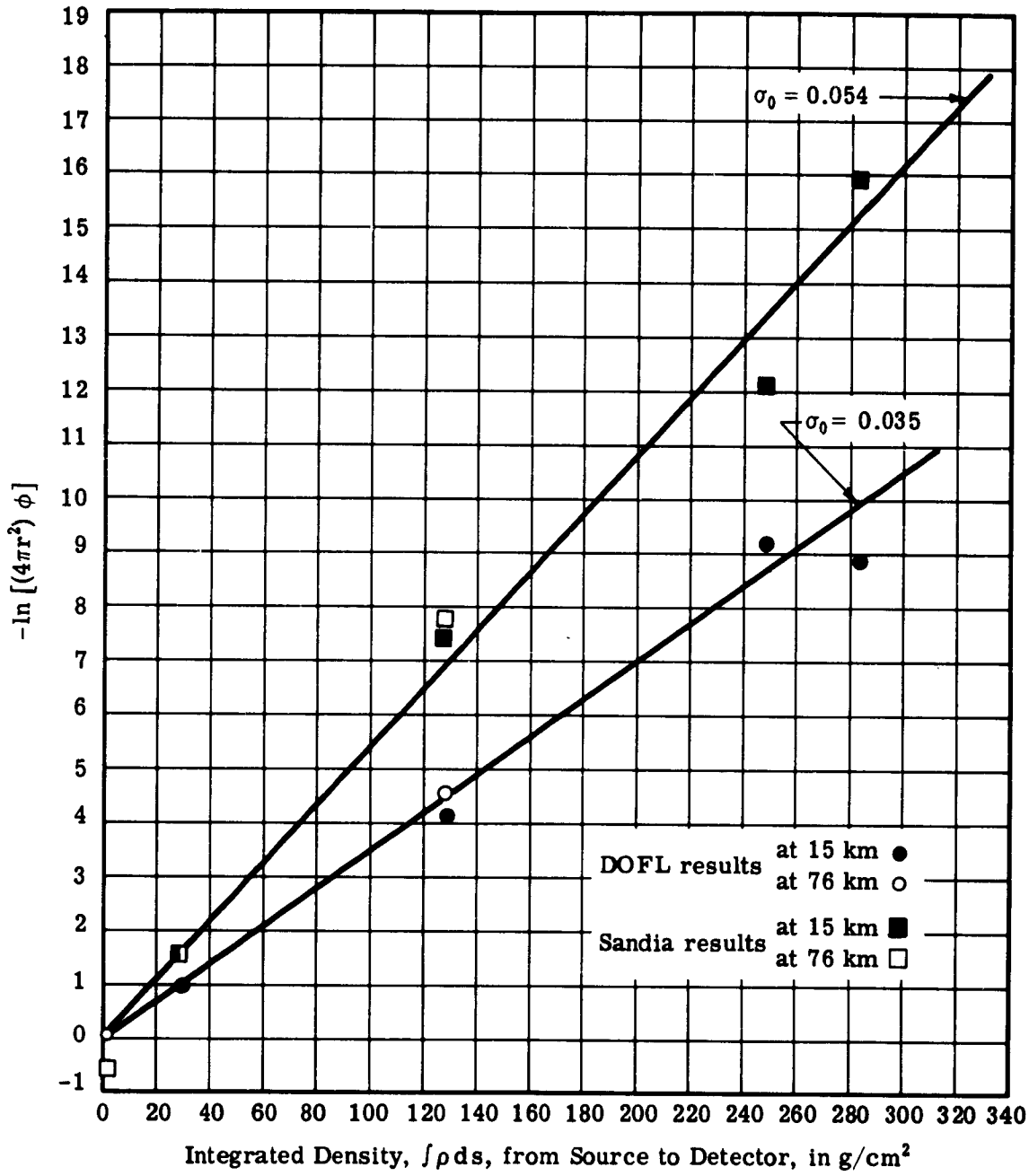


Fig. 2.2 — Neutron penetration in the atmosphere; flux of 10 to 14 Mev neutrons from a 14-Mev source.

Taking Eq. 2.32 for the importance function, an altered transport kernel is defined as before

$$\tilde{T}\ (\underset{\sim}{r}'\rightarrow\underset{\sim}{r}) = \frac{I(\underset{\sim}{r})}{I(\underset{\sim}{r}')}\ \ T(\underset{\sim}{r}'\rightarrow\underset{\sim}{r}) \tag{2.33}$$

$$\frac{I(\underset{\sim}{r})}{I(\underset{\sim}{r}')} = \exp\left\{\frac{\sigma_0}{\gamma}\ [F(z_0) - F(z)] - \frac{\sigma_0}{\gamma'}\ [F(z_0) - F(z')]\right\} \tag{2.34}$$

where

$$\gamma' = \frac{z'}{r'}\ .$$

Aside from necessary delta functions,

$$T(\underset{\sim}{r}'\rightarrow\underset{\sim}{r}\,|\,E')ds = \sigma(E')\rho(z)\ \exp\left\{-\frac{s\sigma(E')}{z-z'}[F(z')-F(z)]\right\}ds \tag{2.35}$$

where $s = |\underset{\sim}{r}-\underset{\sim}{r}'|$ is the distance between $\underset{\sim}{r}$ and $\underset{\sim}{r}'$ as the neutron or gamma flies. Then

$$\tilde{T} = \sigma(E')\rho(z)\ \exp\left\{-\frac{\sigma(E')}{\omega_z'}[F(z')-F(z)]+\frac{\sigma_0}{\gamma}\ [F(z_0)-F(z)]-\frac{\sigma_0}{\gamma'}\ [F(z_0)-F(z')]\right\} \tag{2.36}$$

where $\omega_z' = (z-z')/s$.

We have been unable to devise a T' which resembles $\tilde{T}$ as closely as was done before and which permits an easy determination of the distance to be traveled. If, as before, we set the exponent in $\tilde{T}$ equal to $-\lambda_0$ (chosen from $e^{-\lambda}$) we get a transcendental equation for z:

$$\lambda_0 = -\frac{\sigma(E')}{\omega_z'}\ F(z) + \frac{\sigma_0}{\gamma}\ F(z) + \text{const} \tag{2.37}$$

Note that $\sigma(E')/\omega_z'$ is a constant which is known but γ depends upon z, and that F(z) is approximately exp(-Az). If the last equation is easily solved (e.g., by trial and error), and if $d\lambda/ds \neq 0$, then a scheme like the exponential transformation can be worked out. We have assumed that this would be inconvenient and propose

a direct ad hoc application of the approximate exponential transformations of Eq. 2.27. That is, define a T'' using

$$\sigma(E') - \omega\sigma_0 \text{ for } s \leq r'$$

and

$$\sigma(E') - \sigma_0 \text{ for } s > r';$$

here

$$\omega = \frac{\underset{\sim}{r}' \cdot (\underset{\sim}{r} - \underset{\sim}{r}')}{r's} \tag{2.38}$$

so that

$$T''(s)\, ds = \rho\,(z)[\sigma(E') - \omega\sigma_0]ds \exp\left\{-\frac{\sigma(E')-\omega\sigma_0}{\omega'_z}\,[F(z') - F(z)]\right\}; \quad s \leq r',$$

$$= \rho(z)\,[\sigma(E')-\sigma_0]\, ds \exp\left\{-\frac{\sigma(E')-\sigma_0}{\omega'_z}\,[F(z_1)-F(z)]\right.$$

$$\left. + \frac{\sigma(E')-\omega\sigma_0}{\omega'_z}\,[F(z_0)-F(z_1)]\right\}; \quad s \geq r' \tag{2.39}$$

z_1 is that value of z for which $s = r'$, i.e.,

$$z_1 = z' + \omega'_z\, r' \tag{2.40}$$

To carry this out, pick a λ from $e^{-\lambda}$ and

1. If $\lambda \leq \lambda_1 \equiv [F(z')-F(z_1)]\ \dfrac{\sigma'-\sigma_0\omega}{\omega'_z}$,

z is determined from

$$F(z) = F(z_0) - \frac{\omega'_z\lambda}{\sigma'-\sigma_0\omega} \tag{2.41}$$

and

$$N = \frac{\sigma'}{\sigma'-\omega\sigma_0}\ \exp\left\{-\sigma_0\left(\frac{1}{\gamma'} - \frac{1}{\gamma}\right)[F(z_0) - F(z')] - \left(\frac{\sigma'}{\omega'_z} - \frac{\sigma_0}{\gamma}\right)\frac{\gamma\lambda}{\sigma'-\omega\sigma_0} + \lambda\right\} . \tag{2.42}$$

2. If $\lambda > \lambda_1$, z is determined from

$$F(z) = F(z_1) - \frac{\omega'_z\,(\lambda-\lambda_1)}{\sigma'-\sigma_0}$$

and

$$N = \frac{\sigma'}{\sigma'-\sigma_0}\,\exp\left\{-\sigma_0\left(\frac{1}{\gamma'}-\frac{1}{\gamma}\right)[F(z_0)-F(z')]-\left(\frac{\sigma'}{\omega'_z}-\frac{\sigma_0}{\gamma}\right)\left(\frac{\omega'_z\lambda_1}{\sigma'-\sigma_0\omega}+\omega'_z\frac{\lambda-\lambda_1}{\sigma'-\sigma_0}\right)+\lambda\right\}$$

(2.43)

It is recommended that if N particles are to go into the next collision, and if σ_S/σ_T is the probability of survival, that it be arranged that just N σ_S/σ_T, on the average, come out of the next collision. Naturally, the proper proportion of elastic, inelastic scatterings, and other possible interactions must be preserved.

Finally, some means must be employed to cut off the importance sampling at very large distances so as to prevent particles from wandering out to infinity. A simple method of doing this consists in terminating a history when a particle leaves a large volume which encloses the problem. The cutoff should be sufficiently far from a detector that it has a negligible effect on the flux at that detector.

3. SCORING METHODS – FLUX AT A POINT

3.1 UNCOLLIDED FLUX ESTIMATOR

In some calculations of a radiation field, it is desirable to obtain answers for flux, dose, or the like at a point. The alternative – to estimate similar quantities as averaged over finite volumes – may be satisfactory if some care is used in choosing the volume small enough so that the difference between averaged answer and its point value is small. If this volume is very small, then there is no essential difference from flux at a point.

Since no history can be expected to carry a neutron through a point, it is necessary to use analytic expected value estimates. One common method uses the relation between $\psi(\underset{\sim}{r}', E, \underset{\sim}{\Omega})\, d\underset{\sim}{r}' dE\, d\underset{\sim}{\Omega}$, the density of particles entering collision in volume $d\underset{\sim}{r}$ with energy in dE and direction in $d\underset{\sim}{\Omega}$, and the flux at $\underset{\sim}{r}$:

$$\phi(\underset{\sim}{r}) = \int dE' \int d\underset{\sim}{r}' \int dE \int d\underset{\sim}{\Omega}\, \psi(\underset{\sim}{r}', E, \underset{\sim}{\Omega}) \times \left\{ 2g\left[\frac{\underset{\sim}{r}-\underset{\sim}{r}'}{|\underset{\sim}{r}-\underset{\sim}{r}'|} \cdot \underset{\sim}{\Omega};\ E \right] \times \frac{e^{-\mu(E')\,|\underset{\sim}{r}-\underset{\sim}{r}'|}}{4\pi\,|\underset{\sim}{r}-\underset{\sim}{r}'|^2} \right\} \tag{3.1}$$

In this expression $g(\omega, E)\, d\omega$ is the probability of scattering a neutron of energy E through an angle whose cosine is in the range $(\omega, \omega + d\omega)$. E′ is the energy after scattering and $\mu(E')$ is the total attenuation coefficient of the scattered neutron. Isotropic scattering gives

$$g = \frac{1}{2}\,\frac{\sigma_S}{\sigma_T}\,. \tag{3.2}$$

The straightforward method of using this expression is to evaluate the estimator in braces every time a particle goes into collision and average over histories.

It is easy to see that this procedure yields an infinite variance if the point $\underset{\sim}{r}$ lies within the medium. In the neighborhood of $\underset{\sim}{r}'$, let $r = |\underset{\sim}{r} - \underset{\sim}{r}'|$; the integral is essentially of the form

$$\overline{\phi} \sim \psi(\underset{\sim}{r}') \int r^2 dr \, \frac{1}{4\pi r^2} \tag{3.3}$$

which converges. The mean square flux has contributions like

$$\overline{\phi^2} \sim \psi(r') \int r^2 dr \left(\frac{1}{4\pi r^2}\right)^2 \tag{3.4}$$

which does not converge.

The fact that the variance is infinite does not necessarily imply that the use of this procedure is improper. Indeed it will be proved that for many histories, the mean value of the flux obtained in this way converges to the correct answer. On the other hand, the analysis shows that the infinite variance method has an error that converges more slowly than if the variance is finite. For this reason it is desirable to find a method which has a finite and reasonably small variance. This section will be devoted to an analysis of the effects of the infinite variance and a discussion of several methods of making the variance finite.

3.2 ANALYSIS OF THE INFINITE VARIANCE ESTIMATOR

According to the previous analysis, the infinity in the variance of the uncollided flux estimator arises from the behavior of the estimator near $r = 0$, namely as r^{-2}. Essentially the same situation should occur if we sample a random variable x with a p.d.f. $\propto x^2$ near the origin and evaluate an estimator proportional to x^{-2}. Let us analyze this situation where, for convenience, the range of x is $(0,1)$.

Suppose

$$p(x) = 3x^2 \quad 0 \leq x \leq 1 \tag{3.5}$$

and the estimator is

$$z(x) = (3x^2)^{-1} \tag{3.6}$$

Clearly

$$\langle z \rangle = \int_0^1 p(x)\, z(x)\, dx = 1$$

$$\langle z^2 \rangle = \int_0^1 p(x)\, [z(x)]^2\, dx = \infty \tag{3.7}$$

To determine the convergence to the mean of the average value of z, let us first find the p.d.f. of z:

$$p_Z(z) = \frac{1}{z}\left|\frac{dx}{dz}\right| = \frac{1}{2\sqrt{3}}\, z^{-5/2}, \quad \frac{1}{3} \leq z < \infty. \tag{3.8}$$

In order to calculate the behavior of the sum of many values of z chosen independently, a knowledge of the characteristic function[6] is required. The latter is

$$ch_Z(t) = \int_{-\infty}^{\infty} e^{izt} p_Z(z)\, dz = \frac{1}{2\sqrt{3}} \int_{1/3}^{\infty} z^{-5/2}\, e^{izt} dz \tag{3.9}$$

This integral is not easy to determine in closed form. However, its behavior near the origin may be computed. Let

$$h(t) = t^{-3/2}[ch_Z(t) - 1 - it] \tag{3.10}$$

$$= t^{-3/2} \int_{1/3}^{\infty} \frac{1}{2\sqrt{3}}\, \frac{e^{itz} - 1 - itz}{z^{5/2}}\, dz$$

$$= \frac{1}{2\sqrt{3}} \left[\int_0^{\infty} \frac{e^{iu} - 1 - iu}{u^{5/2}} \, du - \int_0^{t/3} \frac{e^{iu} - 1 - iu}{u^{5/2}} \, du \right] \tag{3.11}$$

Now, since the integrand behaves like $u^{-1/2}$ near the origin, the first integral exists and the second is proportional to $t^{1/2}$. Thus, near $t = 0$,

$$ch_Z(t) = 1 + it + \gamma t^{3/2} + \delta t^2 + \ldots \tag{3.12}$$

$$\log ch_Z(t) = it + \gamma t^{3/2} + \delta' t^2 + \ldots$$

Suppose a z is computed independently n times, and

$$Z = \sum_{i=1}^{n} z_i \tag{3.13}$$

$$ch_Z(t) = \prod_{i=1}^{n} ch_{Z_i}(t) = [ch_z(t)]^n \tag{3.14}$$

$$\log ch_Z(t) = n \log ch_z(t) = int + \gamma nt^{3/2} + \delta' nt^2 + \ldots \tag{3.15}$$

When a linear change is made in a random variable:

$$\zeta = a + bZ \tag{3.16}$$

we get

$$ch_\zeta(t) = \int e^{it\zeta} \, p_\zeta(\zeta) \, d\zeta$$

$$= \int e^{it(a+bZ)} p_Z(Z) dZ$$

$$= e^{ita} ch_Z(bt) \tag{3.17}$$

Then if we put

$$\zeta = \frac{Z/n - 1}{n^{-1/3}} = -n^{1/3} + n^{-2/3} \, Z \tag{3.18}$$

$$\log ch_\zeta(t) = -in^{1/3}t + in\,(n^{-2/3}t) + \gamma n\,(n^{-2/3}t)^{3/2} + \delta' n(n^{-2/3}t)^2 + \ldots$$

$$= \gamma t^{3/2} + \delta' n^{-1/3} t^2 + \ldots \tag{3.19}$$

In the limit $n \to \infty$,

$$\log \mathrm{ch}_\zeta(t) = \gamma t^{3/2} \tag{3.20}$$

The inversion of this characteristic function leads to a unique p.d.f. for ζ. At the moment, the precise form of this is not important. Note, however, that the relation defining ζ in terms of Z has the form of

$$\zeta = \frac{\overline{z} - \langle z \rangle}{n^{-1/3}} \tag{3.21}$$

where $\overline{z}$ denotes an "experimental" – i.e., Monte Carlo – mean. This means that the difference $\overline{z} - \langle z \rangle$ has expected value zero, its deviation from zero is randomly distributed according to a p.d.f. whose width, as $n \to \infty$, is measured by $n^{-1/3}$. Finally this p.d.f. behaves, for large ζ, as $\zeta^{-5/2}$.

From these results, it may be concluded that in this situation, the fact that the variance is infinite is in itself no reason against its use. The first requirement on any method, that after repeated sampling, it give an answer close to the correct answer, is preserved. On the other hand, its convergence is slower than if the variance exists and large departures from the expected deviation from the mean may occur.

It may be objected that in any actual calculation, it will be necessary to truncate z and that this, in fact, guarantees a finite variance. To investigate this, let us suppose that the c.d.f. of z is truncated in the following way:

$$P_{tz}(z) = \frac{1}{2\sqrt{3}} \int_{1/3}^{z} z'^{-5/2}\, dz' = 1 - \frac{1}{3\sqrt{3}}\, z^{-3/2}; \quad \frac{1}{3} \leq z \leq z_0,$$

$$P_{tz}(z) = 1 - \frac{1}{3\sqrt{3}}\, z_0^{-3/2}; \quad z_0 \leq z < 3z_0, \tag{3.22}$$

$$P_{tz}(z) = 1; \quad 3z_0 \leq z < z_0.$$

The step at $3z_0$ is arranged so that

$$\int_{1/3}^{\infty} z dP_{tz}(z) = 1$$

Then it is easy to see that $<z^2> \propto z_0^{1/2}$, $<z^3> \propto z_0^{3/2}$. By computing the characteristic function of z, and of $Z = \Sigma z_i$ and finally of

$$\zeta_t = \frac{Z}{n^{1/2}} - n^{1/2}$$

it is possible to show that, although the variance is finite ($\propto z_0^{1/2}$), it requires a sample size at least as large as $n \gtrsim z_0^{3/2}$ before the distribution of the mean becomes normal. This supports the intuitive expectation that truncation does not help as long as the expected number of samples in the truncated part of the distribution is small. In other words, if the truncation is to do any good, it must have an appreciable effect on the average result.

To return to the estimation of flux at a point, we note that the truncation can be carried out. At best, however, it results in estimation of average flux over a small region. The argument above shows that this region should be chosen so that an appreciable number of collisions take place inside it during the actual sampling if the benefits of finite variance are to be felt. This, of course, leads to the same dilemma in choosing volumes as one has in the first place.

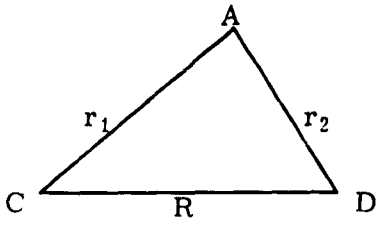
3.3 FINITE VARIANCE METHODS

As a general rule, to reduce the variance of the Monte Carlo estimate of an integral it is desirable to sample from a density function which resembles, as closely as possible, the entire integrand. If the integrand includes any singular part, it should be incorporated in the sampling p.d.f., not in the scoring function.

In the flux estimation, the singularity (in the second moment) derives from the r^{-2} behavior of the estimator. If this is to be removed, the p.d.f. which determines the point at which the collision occurs (the collision from which the flux estimate is made), must be altered so as to include explicitly the r^{-2}. This means in turn that these last collisions before estimation cannot occur in the usual way.

What is required is that for every collision, we estimate the "once-more collided" contribution to the flux at a point, and choose the position of the intermediate collision so as to make the variance finite. If this procedure is carried out for every collision – including the source – then the final estimate is for collided flux only. A separate analytic calculation must be made of the uncollided flux.

To determine a suitable p.d.f. for the intermediate collision point, we consider the integral for the once scattered flux at a detector a distance R away from a collision. Assume, for simplicity, that scattering is isotropic, that the cross section is unchanged by collision and that the scattering probability is C.



The sketch shows the geometry with the collision at point C, the detector at D. The once scattered flux at D, given that a particle goes into* collision at C is

$$\phi_1 = C^2 \int dV \frac{e^{-\mu r_1}}{4\pi r_1^2} \frac{e^{-\mu r_2}}{4\pi r_2^2} \tag{3.23}$$

The singularity in the variance may be removed if the p.d.f. of the intermediate point A contains the factor $dV/r_1^2 r_2^2$. Both radii are needed; if only r_2^2 is used, then the collision points occurring close to C would again give infinite variance. The simplest such distribution is

$$U_1(R)\, dV = \frac{R}{\pi^3} \frac{dV}{r_1^2 r_2^2} \tag{3.24}$$

---

*Note that if a particle is known to come out of a collision at C, as for example in the source, the factor C^2 in this integral is replaced by C.

If the intermediate point is sampled from $U_1(r)$, then the flux estimator is

$$f_1 = \frac{C^2}{U_1} \frac{e^{-\mu(r_1+r_2)}}{(4\pi)^2 r_1^2 r_2^2} = \frac{\pi C^2}{16} \frac{e^{-\mu(r_1+r_2)}}{R} \tag{3.25}$$

We note that when C falls close to D, R becomes small and f_1 large. However, since the singularity is only R^{-1}, the mean square of f_1 exists. Higher moments of f_1 diverge. This fact does not negate the usual form of the central limit theorem but it means that Monte Carlo estimates of the variance itself are more than usually uncertain. Moreover, the convergence to the normal law will be slower than if $<f_1^3>$ existed. Higher moments of the scattering may be made to converge by including more orders of scattering in the estimation process.

Although U_1 removes the difficulty associated with small r_1 or r_2, its behavior for large r_1 and r_2 is not very close to the behavior of the integrand of the single scattering integral. The following* p.d.f. may be better in that respect:

$$U_2 dV = \frac{\mu'}{8\pi} \left[\frac{e^{-\mu' r_1}}{r_1^2} + \frac{e^{-\mu' r_2}}{r_2^2} \right] dV \tag{3.26}$$

For fixed R and r_2 small,

$$U_2 \approx \frac{\mu'}{8\pi} \left[\frac{r_1^2 + r_2^2 e^{-\mu' R}}{r_1^2 r_2^2} \right] \approx \frac{\mu'}{8\pi} \frac{1}{r_2^2} \tag{3.27}$$

This shows that, again for fixed R, the use of U_2 makes the single scattering integration have finite variance.

For R small the mean square may be shown to vary as

$$\overline{\Phi}^2 = \frac{1}{\mu' R^3} \tag{3.28}$$

As we integrate over R with weight factor R^2, the final integral diverges unless μ' is made to vary as $1/R$ for small R. Up to now μ' is arbitrary so that it may be made a function of R such that

*We are limiting the choice of U to functions for which the choice is straightforward.

$$\lim_{R \to 0} R\mu'(R) \tag{3.29}$$

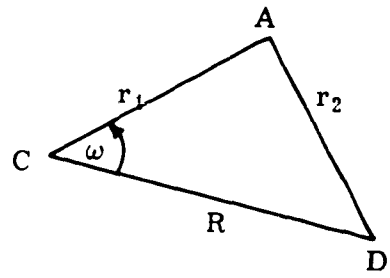
exists. For example, we may use

$$\mu' = \mu + \frac{1}{R} . \tag{3.30}$$

3.4 SAMPLING FROM $U_1(r)$ AND $U_2(r)$

To pick a point from

$$U_1(r)\, dV = \frac{R}{\pi^3} \frac{dV}{r_1^2 r_2^2} ,$$



use ω and r_1 as coordinates; ω is the cosine of the angle between $\underset{\sim}{r}_1$ and $\underset{\sim}{R}$.

Then write

$$U_1(r_1,\omega)\, dV = \left\{ \frac{U_1(r_1,\omega)\, d\omega\, d\varphi}{\int_{-1}^{1} d\omega \int_0^{2\pi} d\varphi\, U_1(r_1,\omega)} \right\} \int_{-1}^{1} d\omega \int_0^{2\pi} d\varphi\, U_1(r_1,\omega) r_1^2 dr_1 \tag{3.31}$$

The integral

$$M(r_1) = r_1^2 \int d\omega \int d\varphi\; U_1(r_1,\omega) \tag{3.32}$$

is the marginal distribution for r_1. If we pick an r_1 from $M(r_1)\, dr_1$, then the quantity in brackets is a conditional distribution for ω and φ given r_1.

A straightforward integration shows that

$$M(r_1) = \frac{2}{\pi^2} \frac{1}{r_1} \log \frac{r_1+R}{|r_1-R|} \tag{3.33}$$

If we set

$$r_1 = R_1 y,$$

then the p.d.f. of y is

$$M_y(y) = \frac{2}{\pi^2}\,\frac{1}{y}\,\log\frac{1+y}{|1-y|};\quad 0 \leq y < \infty \tag{3.34}$$

To pick from this function, note that

$$\int_Y^\infty M_y(y)\,dy = \int_0^{1/Y} M_y(y')\,dy' \tag{3.35}$$

and, in particular,

$$\int_1^\infty M_y(y)\,dy = \int_0^1 M_y(y)\,dy \tag{3.36}$$

Together the last two equations show that to pick y on the range $(0,\infty)$ we may pick a y′ from $M_y(y')$ on (0,1) and with probability 1/2 set $y = y'$, otherwise $y = 1/y'$.

To pick, in turn, on the range (0,1), the function $Y(\xi)$ defined by

$$2\int_0^Y M_y(y)\,dy = \xi \tag{3.37}$$

was tabulated and fitted by a rational fraction:

$$Y(\xi) = \frac{1.2337\,\xi - 0.412593\,\xi^2}{1 - 0.17889\,\xi^2} \tag{3.38}$$

The maximum relative error is 0.002, which seems adequate.

When y is found, ω must be chosen from the p.d.f.

$$w(\omega) = \frac{2\pi R U_1(r_1,\omega)\,r_1^2}{M_y} = \frac{y}{\log\frac{1+y}{|1-y|}}\;\;\frac{1}{1+y^2-2y\omega} \tag{3.39}$$

The solution of

$$\frac{y}{\log \frac{1+y}{|1-y|}} \int_{-1}^{\omega} \frac{1}{1+y^2-2\omega' y} \, d\omega' = \xi \tag{3.40}$$

is

$$\omega = \frac{1+y^2-(1+y)^2[(1-y)^2/(1+y)^2]^{\xi}}{2y} \tag{3.41}$$

and

$$r_2 = \sqrt{r_1^2+R^2-2r_1R\omega} = R(1+y) \left|\frac{1-y}{1+y}\right|^{\xi} \tag{3.42}$$

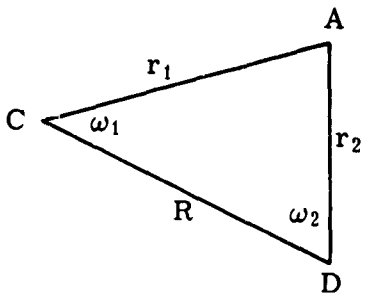
If necessary, an azimuthal angle may be chosen (at random) so as to specify A, the point of intermediate collision, completely.

To pick from U_2, note that U_2 is an average of two p.d.f.'s each of which has the form

$$\frac{\mu'}{4\pi} \frac{e^{-\mu' r}}{r^2}$$

Picking from U_2 consists simply of the following: (a) pick (with equal probability) either the collision point or the detector point as an origin; (b) pick a direction isotropically; and (c) pick a distance r along that direction from the p.d.f. $\mu' e^{-\mu' r}$. This distance is either r_1 or r_2 and the remaining distance must be computed.

The advantages in using U_2 are that it is easy to sample, and that it is possible to generalize in a straightforward way. We may use various linear combinations of a function of (r_1, ω_1) and a function of (r_2, ω_2). Including ω dependence means that the direction from either origin is chosen in a biased fashion.



Note that if the once collided estimator, $f_1(r_1,r_2)$ is a symmetric function of r_1 and r_2 (as it is for the one velocity isotropic scattering case described above), the following simplification occurs:

$$\int dV\, U_2(r_1,r_2)\, f(r_1,r_2) = \frac{\mu'}{8\pi} \int dV \left[\frac{e^{-\mu' r_1}}{r_1^2} + \frac{e^{-\mu' r_2}}{r_2^2} \right] f_1(r_1,r_2) \qquad (3.43)$$

$$= \frac{\mu'}{8\pi} \int dV\, \frac{e^{-\mu' r_1}}{r_1^2} f_1(r_1,r_2) + \frac{\mu'}{8\pi} \int dV\, \frac{e^{-\mu' r_2}}{r_2^2} f_1(r_2,r_1)$$

$$- \frac{\mu'}{4\pi} \int dV\, \frac{e^{-\mu' r_1}}{r_1^2} f_1(r_1,r_2) \qquad (3.44)$$

This means that the choice of points C or D as an origin may be dispensed with.

3.5 TESTS OF FLUX ESTIMATORS

A series of computer experiments was run in an attempt to compare the results of the different methods of scoring. The problem solved was the collided flux distribution, ϕ_c, in an infinite homogeneous medium which scatters isotropically. For a point isotropic source, accurate numerical solutions are known.[7] A code was set up to generate histories in a completely straightforward way. That is, no importance sampling or other biasing was introduced. Four alternative scoring methods were used:

1. Uncollided flux estimator: $\dfrac{e^{-\mu r}}{4\pi r^2}$

2a. Once collided flux estimator, using U_1

2b. Once collided flux estimator, using U_2

3. Estimating flux from the average track length per unit volume in a thin shell.

The answers for the collided flux are shown in Table 3.1, along with the following additional data: the time per history, the number of histories, the experimental estimate of the standard deviation. The more elaborate methods, 2a and 2b, take more time per history, but seem to have smaller standard deviations for a fixed number of histories. A criterion which combines the two effects is derived from the quantity

$$Q = T \times (\text{variance}), \tag{3.45}$$

the product of the total time by the square of the standard deviation. This parameter should be, on the average, independent of the number of histories, and show whether a more time-consuming method pays off in more accurate answers. This Q is also tabulated for methods 2 and 3. In method 1, the variance is infinite and Q has no meaning.

It requires considerable sampling to get a variance estimate that is accurate enough to draw good curves of Q as a function of distance and for different sampling methods. The results obtained were not generally as accurate as might be desired. Nevertheless we believe that the trends shown are correct. Method 2a seems best, with 2b somewhat, although not much, worse. Method 3 (track length in a thin shell) generally has the largest Q. For C = 0.9 the differences are not great and in two problems, method 3 was better. It should be recalled, however, that in method 3, an entire shell was used to obtain answers. That is, full use was made of the symmetry of the problem. This is entirely justified in the test problem, but not in any calculation without the symmetry. Substantially more time would be required to get answers to this accuracy in a small area on the surface of the shell so as to approximate a point. To be more specific, suppose that a sampling area of 1 (mean free path)^2 on the surface is used. Then it would take $4\pi r^2$ times as long, without biasing, to get equal statistical precision as compared

Table 3.1 — Flux at a Point – A Comparison of Several Methods

Method	$\sigma_S/\sigma_T = C$	r, Source to Detector Distance	Total Number of Histories ≡ N	$\bar{\phi}_c$	Standard Deviation ≡ σ	Time (min/hist.)	Quality ≡ $\sigma^2 t$	$4\pi r^2 Q_s$	Expected Flux ≡ $<\phi_c>$
1	0.9	0.5	2,000	0.25344	-	0.18	-		0.2897
2	0.9	0.5	1,000	0.28795	0.00769	0.375	0.0222		0.2897
2a	0.9	0.5	1,000	0.28384	0.00737	0.405	0.0220		0.2897
3	0.9	0.5	4,000	0.28587	0.01173	0.17	0.0936	0.294	0.2897
1	0.9	1	2,000	0.10981	-	0. 20	-		0.1140
2	0.9	1	1,000	0.11563	0.00562	0.375	0.0118		0.1140
2a	0.9	1	1,000	0.10663	0.00432	0.405	0.00756		0.1140
3	0.9	1	2,000	0.10803	0.00320	0.17	0.00347	0.044	0.1140
1	0.9	2	2,000	0.02916	-	0.20	-		0.03443
2	0.9	2	1,000	0.03173	0.00215	0.375	0.00173		0.03443
2a	0.9	2	1,600	0.03193	0.00220	0.405	0.00312		0.03443
3	0.9	2	2,000	0.03332	0.00119	0.17	0.00043	0.0214	0.03443
1	0.9	3	2,000	0.01088	-	0.20	-		0.01370
2	0.9	3	1,000	0.01166	0.00115	0.375	0.000498		0.01370
2a	0.9	3	1,640	0.01369	0.00184	0.405	0.002246		0.01370
3	0.9	3	2,000	0.01699	0.00240	0.17	0.00195	0.220	0.01370
1	0.3	0.5	12,000	5.603×10^{-2}	-	0.030	-		0.05216
2	0.3	0.5	2,000	5.268×10^{-2}	6.37×10^{-4}	0.073	5.95×10^{-5}		0.05216
2a	0.3	0.5	1.000	5.303×10^{-2}	8.80×10^{-4}	0.082	6.35×10^{-5}		0.05216
3	0.3	0.5	4,000	7.340×10^{-2}	2.29×10^{-2}	0.025	5.23×10^{-2}	0.164	0.05216
1	0.3	1	10,000	1.398×10^{-2}	-	0.033	-		0.01386
2	0.3	1	5,000	1.391×10^{-2}	1.39×10^{-4}	0.070	6.75×10^{-6}		0.01386
2a	0.3	1	1,000	1.361×10^{-2}	2.72×10^{-4}	0.082	6.07×10^{-6}		0.01386
3	0.3	1	2,000	1.340×10^{-2}	1.28×10^{-3}	0.025	8.15×10^{-5}	1.02×10^{-3}	0.01386
1	0.3	2	2,000	2.284×10^{-3}	-	0.031	-		0.002164
2	0.3	2	1,000	1.990×10^{-3}	6.22×10^{-5}	0.077	2.98×10^{-7}		0.002164
2a	0.3	2	1,600	2.152×10^{-3}	6.66×10^{-5}	0.082	5.81×10^{-7}		0.002164
3	0.3	2	2,000	2.005×10^{-3}	2.02×10^{-4}	0.024	1.97×10^{-6}	9.9×10^{-5}	0.002164
1	0.3	3	2,000	4.069×10^{-4}	-	0.030	-		4.766×10^{-4}
2	0.3	3	1,000	4.422×10^{-4}	1.58×10^{-5}	0.075	1.87×10^{-8}		4.766×10^{-4}
2a	0.3	3	2.400	5.039×10^{-4}	2.58×10^{-5}	0.082	1.31×10^{-7}		4.766×10^{-4}
3	0.3	3	2,000	4.599×10^{-4}	6.21×10^{-5}	0.024	1.85×10^{-7}	2.09×10^{-5}	4.766×10^{-4}

with the situation where the whole shell is used. This increases Q by a factor of $4\pi r^2$. The result is shown in the last column. This Q is much larger than the others.

In judging the usefulness of alternative scoring schemes in other codes, some care must be used in interpreting these results. In the tests, the time required to generate a single collision was relatively short. In a code in which a larger fraction of time is devoted to tracking, the more elaborate and slower methods, 2a and 2b, would show up better. In a code in which there were many detectors and every collision was used to obtain an estimate at every detector, the reverse would be true. We believe that this is not a sensible thing to do; the next section discusses the alternatives.

Unfortunately it is not possible to use a simple criterion like Q to compare estimation method 1 with the others. Nevertheless, we note that almost all the calculations were arranged so that the same time was used in a method 1 run as in a method 2. With one or two exceptions, the deviation from the right answer is much larger in 1. As we have seen, the infinite variance method converges more slowly so that additional sampling will enlarge the difference.

Fig. 3.1 shows a comparison of cumulative averages of flux at a point as given by methods 1 and 2a. The results are for a problem with C = 0.3 and a point 0.5 mean free paths from the source. We see that the method 1 averages are consistently poorer by far and furthermore are scarcely better after many thousand histories than after a few hundred.

On this basis it is recommended that method 2a or 2b be used if flux at a point must be determined. The experiments show 2a better than 2b, at least in the version of the latter that was used. Until a better method along the lines of 2b is worked out, we suggest use of 2a.

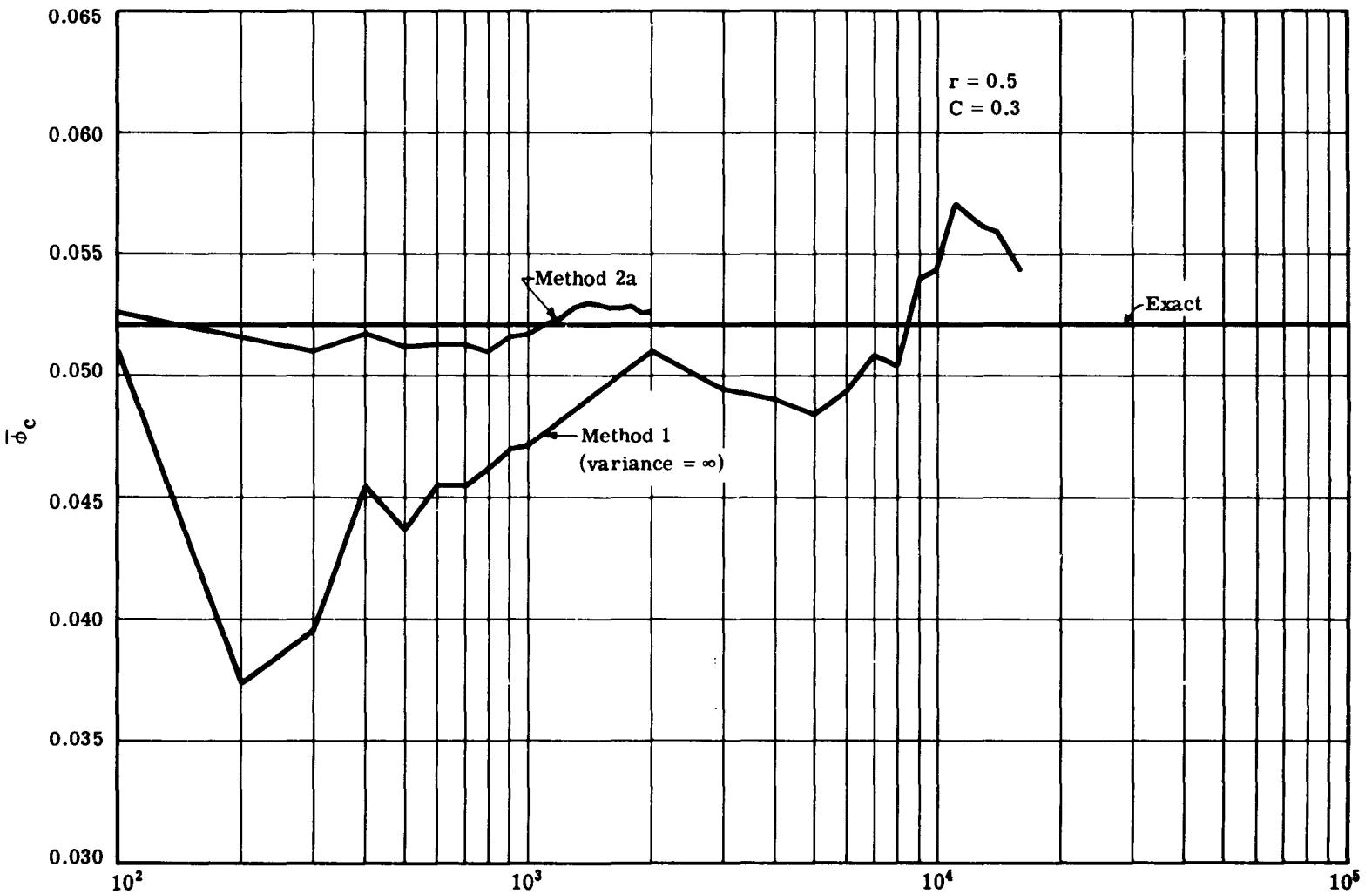


Fig. 3.1 — Cumulative average collided flux after n histories

4. FLUX ESTIMATION AT RANDOM

In calculating the radiation field of a weapon, it is likely that answers at many detectors would be required. Suppose that a flux estimation method is used that gives an answer for every collision. It is then possible, or even likely, that a large part of the computation time will be taken up with this flux estimation. Much of this time will be wasted, since any given collision will generally be far from most of the detectors. The partial answers at these detectors will be very small, and the computation time used would be better used following more histories.

It appears to be desirable, then, to cut off the flux estimation process at large distances. One way of doing this would be simply not to carry out the estimation when the separation of collision and detector is larger than a certain number of mean free paths. This results in a consistent underestimation of the flux, but if the cutoff is at a sufficiently large distance the error becomes small.

Alternatively, we may choose to carry out the flux estimation with a probability which is a function of collision-detector separation. That is, let R be this separation and let $q(\mu R) \leq 1$ be the probability of making an estimate. If q becomes small as μR becomes large, then a cutoff is accomplished. It seems plausible that q should be very close to 1 for small argument (say within a mean free path) and decrease monotonically.

Suppose that when a particle goes into collision at $\underset{\sim}{P}$ an estimate $f(\underset{\sim}{P})$ is made for a particular flux. Then the average answer is

$$\langle f \rangle = \int \psi\,(\underset{\sim}{P})\, f(\underset{\sim}{P})\, d\underset{\sim}{P} \tag{4.1}$$

If we carry out the estimate with probability of $q(\underset{\sim}{P})$ then the estimate is $f(\underset{\sim}{P})/q(\underset{\sim}{P})$ so that

$$\langle f \rangle = \int \psi\,(\underset{\sim}{P})\; q(\underset{\sim}{P})\; [f(\underset{\sim}{P})/q(\underset{\sim}{P})]\; d\underset{\sim}{P}. \tag{4.2}$$

The mean square answer is

$$\langle f^2 \rangle = \int \psi\,(\underset{\sim}{P})\; \frac{f^2(\underset{\sim}{P})}{q(\underset{\sim}{P})}\, d\underset{\sim}{P} + \int d\underset{\sim}{P}\; \psi(\underset{\sim}{P})\; f(\underset{\sim}{P}) \int d\underset{\sim}{P}'\, \psi(\underset{\sim}{P}' \mid \underset{\sim}{P})\; f(\underset{\sim}{P}') \tag{4.3}$$

where $\psi(\underset{\sim}{P}' \mid \underset{\sim}{P})$ is the collision density at $\underset{\sim}{P}'$ given that a collision took place at $\underset{\sim}{P}$. Clearly

$$\psi(\underset{\sim}{P}' \mid \underset{\sim}{P}) = C(E \to E', \underset{\sim}{\Omega} \to \underset{\sim}{\Omega}' \mid \underset{\sim}{r})\; T\,(\underset{\sim}{r} \to \underset{\sim}{r}' \mid E', \underset{\sim}{\Omega}') \tag{4.4}$$

Eq. 4.3 shows that $\langle f^2 \rangle$ and hence the variance in one history are smallest if $q = 1$ throughout. On the other hand the computing time is

$$T = T_0 + t_1 \int \psi(\underset{\sim}{P})\, q(\underset{\sim}{P})\; d\underset{\sim}{P} \tag{4.5}$$

where T_0 is the time for tracing the histories and computing and testing q. Since the time decreases as q is made smaller, and since our general aim is to minimize variance times time, it is possible that $q \not\equiv 1$ is optimum.

The determination of the best q from Eqs. 4.4 and 4.5 appears very difficult. In the brief work devoted to this aspect of scoring, we have used simple functional forms for q, each containing an adjustable parameter.

The work on comparing various scoring methods for flux at a point showed that it requires very lengthy sampling (at least on a Datatron) to compute relative variances accurately. We tried, therefore, to study the effects of using q analytically.

For a straight ahead transport problem with absorption, the flux satisfies

$$\frac{d\phi}{dx} + \mu\phi = C\,\mu\phi$$

with the solution

$$\psi = \mu\phi = \mu e^{-(1-C)\mu x}.$$

We may use ψ together with the estimates for the current at X

$$f = C e^{-\mu(X-x)}$$

and

$$q = e^{-\beta\mu(X-x)} \tag{4.6}$$

in order that the integrals in Eqs. 4.3 and 4.5 may be done analytically.

In this way it is possible to study the behavior of Q (variance × time) as a function of C, μx, and β.

For a hypothetical problem with many detectors, a weighted average of the individual variances is used instead of a single variance. If V_i is the variance at the i^{th} detector (at X_i) then the efficiency is computed from

$$Q = \left(\Sigma \frac{V_i}{<f_i>^2}\right) T$$

and the time includes flux estimation for each detector.

The results will not be shown in detail since they are not extensive enough for interpretation and apply to a model probably too artificial to believe. They indicate, however, that savings on the order of a factor of 1.4 to 5 might be achieved. The larger factor is associated with many detectors.

A similar calculation was carried out with a collision density altered by importance sampling. The general conclusion is the same: by proper choice of β, savings of a factor of up to about 10 might be expected.

It was apparent in both of these that the detailed results are sensitive to the details of the assumptions of distribution of collisions, as well as q and so on. Apart from the suggestion that the method is worth pursuing further, we believe that more useful conclusions may not be drawn.

In an effort to apply the idea to a more realistic case, one machine code for estimating flux at a point was modified to carry out the scoring at random. For this work the function

$$(q\mu R) = \frac{1}{1 + (\beta\mu R)^2} \tag{4.7}$$

was used.

This q has two advantages. For one, it falls below one slowly near R = 0. Secondly, it makes the computation of variance as a function of β easier. From Eq. 4.3 we see that the variance must have the functional form

$$V = A + B\beta^2$$

By plotting experimental variances as a function of β^2 it is possible to determine a reasonable straight line in spite of fluctuations. See Fig. 4.1. It is straightforward to determine the computing time as a function of β as in Fig. 4.2. The times shown refer to the computation for a single detector, but the average time for collision mechanics may be found. From this the time for a many detector problem (with each detector the same distance from the source) may be computed. The Q is shown in Figs. 4.3 and 4.4 for one and 10 detectors, respectively, all two mean free paths from the source. The savings are at most about 24% which is not very encouraging. However, since the penetrations are not very great, not much should be expected.

The potential of the notion of doing the flux calculation at random remains to be proved. It would be best to try the experiments in a code nearly like the final transport code. In view of the many possibilities of choice of q, it would be very desirable to get some insight, if only qualitative, of the characteristics of an optimum q. It appears that the method is likely to help shorten the computation.*

*Use of a q may be even more justified in problems in which the flux estimation time increases with collision-detector separation. Any problem with complicated geometry will have this characteristic.

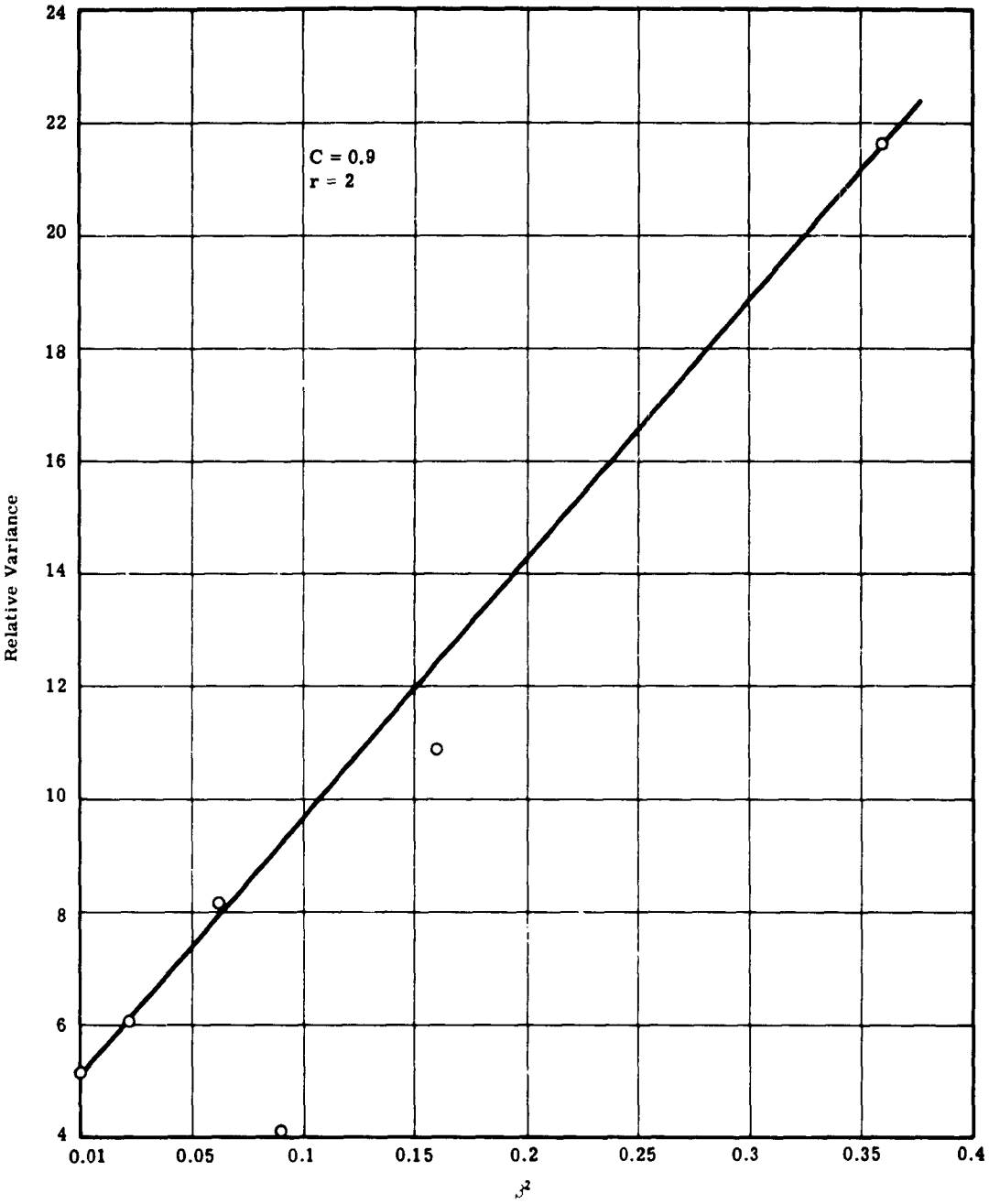


Fig. 4.1 — Flux estimation at random; relative variance for one history vs β^2

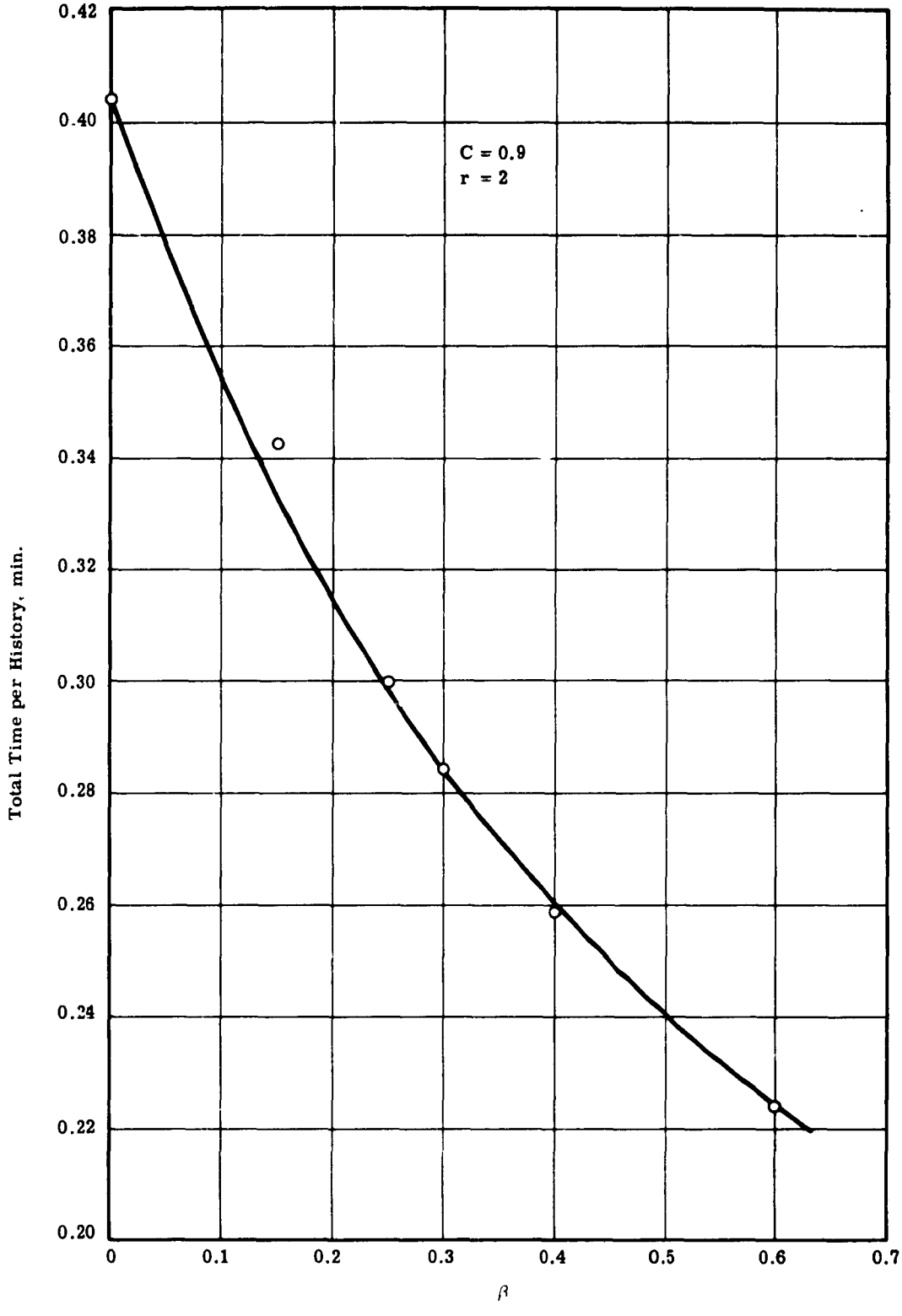


Fig. 4.2 — Flux estimation at random time per history as a function of β

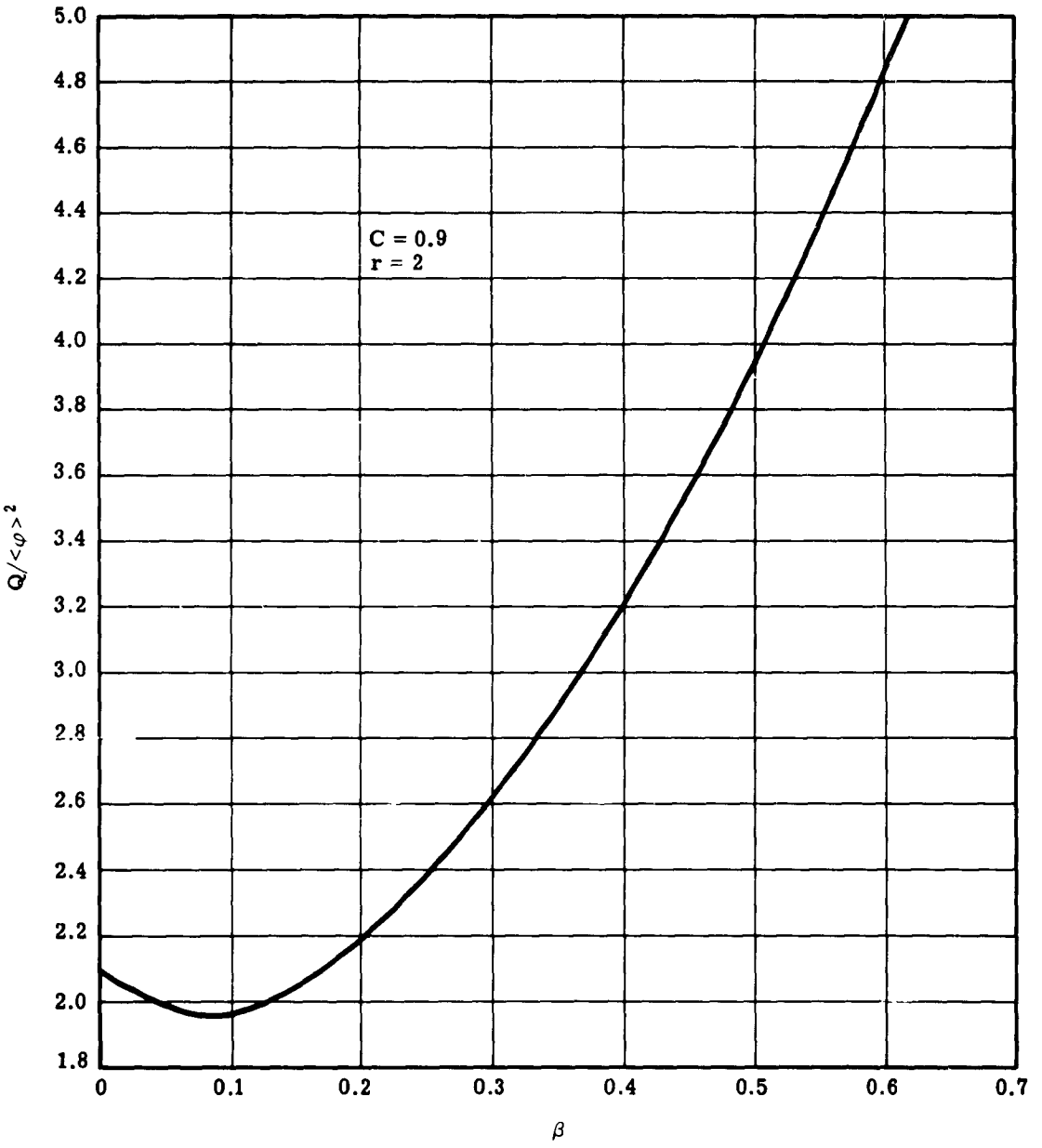


Fig. 4.3 — Flux estimation at random; variance × time for one detector

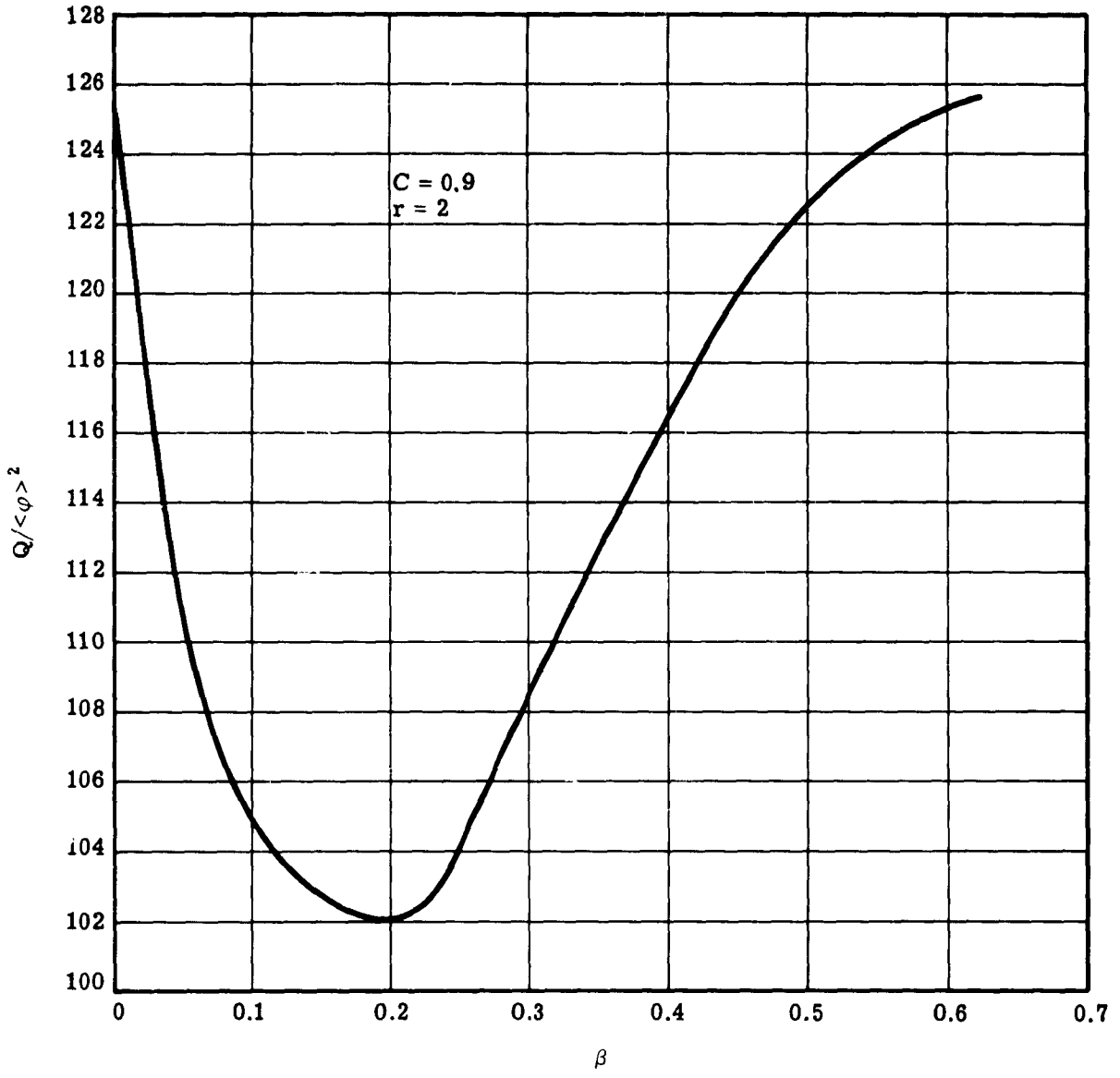


Fig. 4.4 — Flux estimation at random; variance × time for 10 detectors

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